Van Hove singularity and spontaneous Fermi surface symmetry breaking in $Sr_3Ru_2O_7$

Hiroyuki Yamase[1] and Andrey A. Katanin[1,2]

[1]*Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*

[2]*Institute of Metal Physics, 620219 Ekaterinburg, Russia*

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Abstract

The most salient features observed around a metamagnetic transition in $Sr_3Ru_2O_7$ are well captured in a simple model for spontaneous Fermi surface symmetry breaking under a magnetic field, without invoking a putative quantum critical point. The Fermi surface symmetry breaking happens in both a majority and a minority spin band but with a different magnitude of the order parameter, when either band is tuned close to van Hove filling by the magnetic field. The transition is second order for high temperature T and changes into first order for low T. The first order transition is accompanied by a metamagnetic transition. The uniform magnetic susceptibility and the specific heat coefficient show strong T dependence, especially a $\log T$ divergence at van Hove filling. The Fermi surface instability then cuts off such non-Fermi liquid behavior and gives rise to a cusp in the susceptibility and a specific heat jump at the transition temperature.

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Usually the symmetry of the Fermi surface (FS) satisfies the point-group symmetry of the underlying lattice structure. However, recently a symmetry-breaking Fermi surface deformation with a d-wave order parameter, where the FS expands along the k_x direction and shrinks along the k_y direction, or vice versa, was discussed in the two typical models for cuprate superconductors, the t-J[1, 2] and Hubbard model[3, 4] on a square lattice. This d-wave type Fermi surface deformation (dFSD) is often called d-wave Pomeranchuk instability, referring to Pomeranchuk's stability criterion for isotropic Fermi liquids.[5] However, the dFSD often takes place even without violating such a criterion, since the dFSD instability is usually first order for low temperature,[6, 7] and it can also happen even for strongly correlated systems such as those described by the t-J model.[1, 2] The dFSD instability is driven by forward scattering processes of electrons close to the van Hove points in the two-dimensional Brillouin zone. As a result, the symmetry of the electronic state is reduced from C_{4v} to C_{2v} while the lattice still retains C_{4v} symmetry as long as no electron-phonon coupling is considered. The dFSD state has the same symmetry as the so-called electronic nematic order, which was widely discussed in the context of charge stripes for cuprates.[8]

Recently such a novel FS instability was reported for the ruthenate compound $Sr_3Ru_2O_7$ in the presence of an external magnetic field.[9] $Sr_3Ru_2O_7$ is a bilayered material with metallic RuO_2 planes where the Ru ions form a square lattice. *Ab initio* calculations[10] showed that the electronic band structure is similar to that for the single layered ruthenate Sr_2RuO_4, a well-known spin-triplet superconductor.[11] The ground state of $Sr_3Ru_2O_7$ is, however, paramagnetic.[12] By applying a magnetic field h, $Sr_3Ru_2O_7$ shows a metamagnetic transition at $h = h_c$, around which non-Fermi liquid behavior is observed in various quantities: resistivity,[13, 14] specific heat,[14, 15, 16] and thermal expansion.[17] This non-Fermi liquid behavior was discussed in terms of a putative metamagnetic quantum critical end point (QCEP) and hence $Sr_3Ru_2O_7$ was often referred to as a system with a metamagnetic QCEP.[18, 19, 20] However, subsequent experiments[9] for ultrapure crystals showed that the hypothetical QCEP was hidden by a dome-shaped phase transition line; a first order transition was confirmed at the edges of the transition line and was accompanied by a metamagnetic transition, while a second order transition was inferred for high temperature T. Grigera *et al.*[9] associated this instability with a spontaneous dFSD. Later Kee and Kim[21] demonstrated a metamagnetic transition due to a first-order dFSD phase transition in a phenomenological model, which they discussed might be relevant to $Sr_3Ru_2O_7$. A

direct experimental evidence of the dFSD, however, has not been obtained so far. Other scenarios, namely, microscopic phase separation due to Coulomb interaction[22] and magnetic domain formation due to long-range dipolar interactions,[23] were also proposed to explain the experimental data for $Sr_3Ru_2O_7$.

In this Letter, in addition to confirming a metamagnetic transition due to a first-order dFSD phase transition as reported by Kee and Kim,[21] we show that the experimental phase diagram for $Sr_3Ru_2O_7$, and the T dependences of the uniform magnetic susceptibility and the specific heat are well captured in terms of the dFSD instability near the van Hove filling, without invoking a putative QCEP. We analyze a simple model with a pure forward scattering interaction driving the dFSD instability in the presence of a magnetic field. We find that when either the majority or minority band is tuned to van Hove filling by the magnetic field, the dFSD instability occurs in both bands, but with a different magnitude of the order parameter. The transition is second order for high T and changes into first order for low T. The first order transition is accompanied by a metamagnetic transition. Both the magnetic susceptibility and the specific heat coefficient show strong T dependences, especially a $\log T$ divergence at van Hove filling. This non-Fermi liquid behavior originates from the van Hove singularity in the density of states of the bare dispersion. The dFSD instability then cuts off such non-Fermi liquid behavior and produces a cusp in the susceptibility and a specific heat jump at the transition temperature.

We investigate the dFSD instability in the presence of a magnetic field on a square lattice. The minimal model reads

$$H = \sum_{\mathbf{k},\sigma} (\epsilon^0_{\mathbf{k}} - \mu)\, n^\sigma_{\mathbf{k}} + \frac{1}{2N} \sum_{\mathbf{k},\sigma,\mathbf{k},\sigma'} f_{\mathbf{k}\mathbf{k}'}\, n^\sigma_{\mathbf{k}} n^{\sigma'}_{\mathbf{k}'} - h \sum_{\mathbf{k},\sigma} \sigma n^\sigma_{\mathbf{k}} \tag{1}$$

where $n^\sigma_{\mathbf{k}} = c^\dagger_{\mathbf{k}\,\sigma} c_{\mathbf{k}\,\sigma}$ counts the electron number with momentum $\mathbf{k}$ and spin σ; $c^\dagger_{\mathbf{k}\,\sigma}$ ($c_{\mathbf{k}\,\sigma}$) is an electron creation (annihilation) operator; μ is the chemical potential; N is the number of lattice sites; h is the magnetic field. For hopping amplitudes t and t' between nearest and next-nearest neighbors on the square lattice, respectively, the bare dispersion relation is given by

$$\epsilon^0_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y\,. \tag{2}$$

The forward scattering interaction driving the spontaneous dFSD has the form

$$f_{\mathbf{k}\mathbf{k}'} = -g\, d_{\mathbf{k}} d_{\mathbf{k}'}\,, \tag{3}$$

with a coupling constant $g \geq 0$ and a d-wave form factor $d_{\mathbf{k}} = \cos k_x - \cos k_y$. This ansatz mimics the structure of the effective interaction in the forward scattering channel as obtained for the t-J[1] and Hubbard model.[3] The model (1) without the magnetic field was extensively studied in Refs. 6 and 7.

We decouple the interaction by introducing a spin-dependent mean field $\eta^\sigma = -\frac{g}{N}\sum_{\mathbf{k}} d_{\mathbf{k}}\langle n^\sigma_{\mathbf{k}}\rangle$ and obtain a renormalized band dispersion $\xi^\sigma_{\mathbf{k}} = \epsilon^0_{\mathbf{k}} + \eta d_{\mathbf{k}} - \mu^\sigma$ with $\eta = \sum_\sigma \eta^\sigma$; the mean fields are determined by minimizing the free energy, which is a even function with respect to η, and a solution of $\eta \geq 0$ is considered. The σ-summed mean filed η enters $\xi^\sigma_{\mathbf{k}}$, and thus a finite η^σ in general induces a finite $\eta^{-\sigma}$. The Zeeman field is absorbed completely in the effective chemical potential $\mu^\sigma = \mu + \sigma h$. Since our Hamiltonian (1) does not allow momentum transfer, the mean-field theory solves our model exactly in the thermodynamic limit.

The magnetization is given by $m = \frac{1}{N}\sum_{\mathbf{k},\sigma}\sigma\langle n^\sigma_{\mathbf{k}}\rangle = \frac{1}{N}\sum_{\mathbf{k},\sigma}\sigma f(\xi^\sigma_{\mathbf{k}})$, and thus the uniform magnetic susceptibility χ is

$$\chi = \frac{\partial m}{\partial h} = -\frac{1}{N}\sum_{\mathbf{k},\sigma} f'(\xi^\sigma_{\mathbf{k}})\,, \tag{4}$$

where $f(x) = 1/(e^{x/T}+1)$ is the Fermi function and f' is its first derivative. The electronic specific heat coefficient $\gamma = C/T$ can be obtained straightforwardly by the second derivative of the free energy with respect to T at fixed μ,

$$\begin{aligned}\gamma \;=\; & -\frac{1}{T^2 N}\sum_{\mathbf{k},\sigma}(\xi^\sigma_{\mathbf{k}})^2 f'(\xi^\sigma_{\mathbf{k}}) \\ & + g\frac{\left(\frac{1}{TN}\sum_{\mathbf{k},\sigma} d_{\mathbf{k}}\xi^\sigma_{\mathbf{k}} f'(\xi^\sigma_{\mathbf{k}})\right)^2}{1+\frac{g}{N}\sum_{\mathbf{k},\sigma} d^2_{\mathbf{k}} f'(\xi^\sigma_{\mathbf{k}})}\,.\end{aligned} \tag{5}$$

The second term Eq. (5) is zero above T_c and leads to a specific heat jump at T_c.

Band structure calculations for $Sr_3Ru_2O_7$[10] yield 6 Fermi surfaces for $h = 0$. We focus on a FS closest to $\mathbf{k} = (\pi, 0)$ and $(0, \pi)$ since the dFSD instability is driven by electrons near the van Hove points on a square lattice; we mimic such a FS by choosing $t'/t = 0.35$. We fix $\mu/t = 1$ and take $g/t = 1$ for numerical convenience, although $Sr_3Ru_2O_7$ is expected to have a much smaller g as we discuss later. We choose t as a unit of energy so that $t = 1$ in this paper. Since the results are symmetric with respect to $h \to -h$ and $\sigma \to -\sigma$, we consider only the case $h \geq 0$.

Figure 1 shows a phase diagram in the plane of applied magnetic field h and temperature

T. The dFSD transition occurs around the van Hove energy of the up-spin band ($h = 0.4$) with a second order transition for high T and a first order one for low T; end points of the second order line are tricritical points. Figure 2(a) shows the h dependence of the order parameter η, together with η^σ, at low T. Both $\eta^\uparrow$ and $\eta^\downarrow$ show a jump at the first order transition point, but with a different magnitude. The magnetization m also shows a jump at the first order phase transition [Fig. 2(b)]. Its upward jump with increasing h is due to a generic consequence of the concavity of the grand canonical potential as a function of h. Hence the first order transition of the dFSD instability is necessarily accompanied by a metamagnetic transition. The FSs at low T are shown in Figs. 2(c) and (d) for $h = 0.3$ and 0.5, respectively. The gray lines are FSs for $g = 0$ and an outer (inner) FS corresponds to the up-spin (down-spin) band; the splitting of these FSs is due to the Zeeman energy. The FS instability drives a deformation of both FSs and typically leads to an open outer FS.

Figure 3 shows the T dependence of χ [Eq. (4)] for several choices of h for $g = 0$. For a small field, χ has a weak T dependence with a broad maximum at relatively high T and becomes constant for low T, i.e. Pauli paramagnetic behavior. As h moves close to the van Hove energy ($h = 0.4$), χ starts to have a strong T dependence and forms a pronounced peak at low temperature. The peak position is pushed down to zero temperature at the van Hove energy, where a $\log T$ divergence appears. Similar behavior is seen when the magnetic field is reduced from a large h to the van Hove energy [inset of Fig. 3(a)]. Defining T^* as the peak position of χ, we thus obtain the V-shaped T^* line shown in Fig. 1; in particular T^* goes to zero at the van Hove energy. This behavior is due to the van Hove singularity of the up-spin band, not due to an underlying quantum critical point. Around van Hove filling, the dFSD instability occurs and produces a cusp in the T dependence of χ as shown in Fig. 3(b). A T^* line is thus not defined inside the symmetry broken phase and the thin dashed line in Fig. 1 represents T^* in the absence of the dFSD.

Figure 1 is very similar to the phase diagram reported by Grigera *et al.*[9] with a first order transition for low T, a second order transition for high T, and a V-shaped T^* line, which crosses the transition line near the tricritical points. In experiments, the T^* line was determined by thermal expansion measurements.[24] While peak positions of the magnetic susceptibility were not studied systematically in experiments,[24] we expect that the magnetic susceptibility shows a similar V-shaped T^* line around the van Hove energy. On the other hand, a strong T dependence of the magnetic susceptibility [Fig. 3(a)] was observed in

experiments;[25] the cusp of χ shown in Fig. 3(b) can be tested. Experimental energy scales are, however, much smaller than in our result. To obtain a comparable $T_c \sim 1$K, the coupling constant g should be reduced substantially. As clarified in Ref. 7, in the weak coupling limit the dome-shaped transition line of the dFSD is characterized by a single energy scale $\epsilon_\Lambda e^{-1/(2\overline{g})}$, where ϵ_Λ is a cutoff energy and $\overline{g} = 2m^* g/\pi^2$ is a dimensionless coupling constant with the effective mass m^* near the van Hove energy. The result in the weak coupling limit was checked to be applicable even for finite g with good accuracy.[7] Therefore the phase diagram in Fig. 1 does not change essentially for a smaller g, which just reduces the energy scale of the dFSD transition line around the van Hove point. The relative position of T^* and $T_c^{\rm tri}$ also does not change appreciably, since T^* has linear dependence of h around the van Hove energy.

The electronic specific heat is calculated exactly in our model [see Eq. (5)]. We first show γ for $g = 0$ in Fig. 4 as a function of T for several choices of h. For a relatively small field, γ shows a peak structure for high T (in a logarithmic scale), but becomes constant for lower T as expected for the normal Fermi liquid. As h moves close to the van Hove energy ($h = 0.4$), the peak position is shifted to lower T and a $\log T$ divergence appears at the van Hove energy. A similar behavior is also seen when h is reduced from a large value to the van Hove energy [inset in Fig. 4(a)]. For a finite g, the dFSD instability produces a jump in the specific heat at the transition temperature as shown in Fig. 4(b). This jump typically becomes larger as h is closer to the van Hove energy. Unlike the situation in the BCS theory, the ratio of the magnitude of the jump $\Delta\gamma$ and the normal state specific heat γ_n at T_c is not a universal value. In particular, in the weak coupling limit T_c scales as $\epsilon_\Lambda e^{-1/(2\overline{g})}$ as discussed above. Since γ shows a $\log T$ dependence at van Hove filling, we obtain $\gamma_n \sim \log T_c \sim \overline{g}^{-1} \propto g^{-1}$, while $\Delta\gamma$ is a certain finite value.

A T dependence of γ very similar to Fig. 4(a) was actually obtained in experiments.[14, 15, 16] The specific heat jump is not observed in experiments, but may require a more precise measurement, which would provide a definite evidence of the second order transition; the authors in Ref. 9 inferred a second order transition from the magnetization and the resistivity measurements.

We have shown that the most salient features observed in $Sr_3Ru_2O_7$ are well captured in terms of the dFSD instability near van Hove filling. In particular, the non-Fermi liquid behavior reported for the T dependence of χ and γ can be associated with the van Hove

singularity, not with a putative QCEP as usually discussed.[18, 19] Around van Hove filling, it is known[26, 27] that various other ordering tendencies develop and probably compete with the dFSD tendency. We may thus allow other interactions such as ferromagnetism and antiferromagnetism in our model to explore more detailed comparison with experimental data as well as the interplay among various ordering tendencies in the presence of the magnetic field. The most interesting future issue is how the anomalous T dependence of the resistivity[13, 14] observed in $Sr_3Ru_2O_7$ above T_c can be understood. A crucial question is whether classical dFSD fluctuations and the van Hove singularity are sufficient to capture the resistivity data or whether quantum critical fluctuations originating from some QCEP are necessary. In the latter case, how is the QCEP related to the dFSD instability and the van Hove singularity that we have discussed in the present paper? Both the chemical potential and the magnetic field have to be fine-tuned to reach a QCEP while it is sufficient for either of them to be tuned to realize van Hove filling. In this sense, a QCEP scenario imposes an additional constraint on $Sr_3Ru_2O_7$.

When this work was complete, we have learned about a recent experimental observation of a large magnetoresistive anisotropy inside the dome-shaped transition line in $Sr_3Ru_2O_7$,[28] consistent with the existence of Fermi surface symmetry breaking in this compound.

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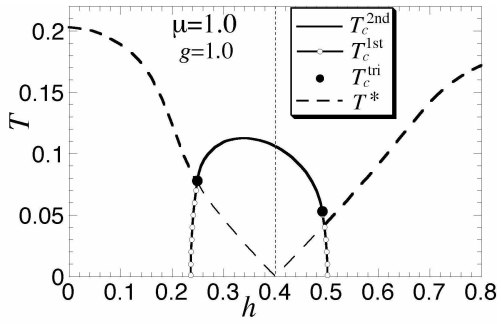

FIG. 1: The dFSD phase diagram in the plane of magnetic field h and temperature T for $\mu = 1.0$ and $g = 1.0$; the transition is second order for high T ($T_c^{\rm 2nd}$) and first order for low T ($T_c^{\rm 1st}$); end points of the second order line are tricritical points ($T_c^{\rm tri}$); the dotted line ($h = 0.4$) represents the van Hove energy of the up-spin band; the dashed line (T^*) denotes a peak position of the uniform magnetic susceptibility and the thin dashed line represents T^* in the absence of the dFSD.

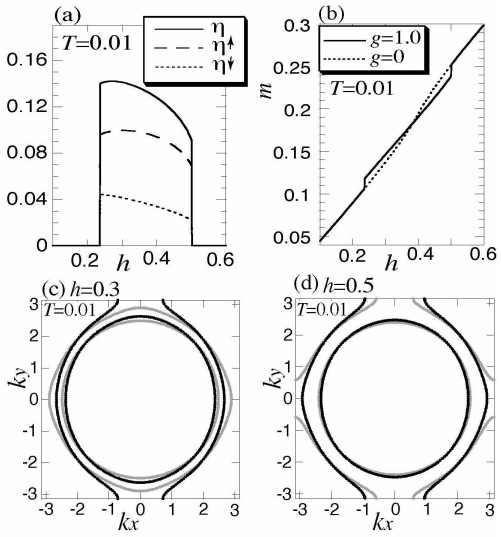

FIG. 2: The mean-field solution at low T for $\mu = 1.0$ and $g = 1.0$. (a) h dependence of the order parameter; note that $\eta = \eta^{\uparrow} + \eta^{\downarrow}$. (b) A metamagnetic transition due to the first order dFSD transition; the result for $g = 0$ is also shown by a dotted line. FSs for $g = 1$ (solid line) and 0 (gray line) at $h = 0.3$ (c) and 0.5 (d); the deformation of the inner FS in (d) is hardly visible.

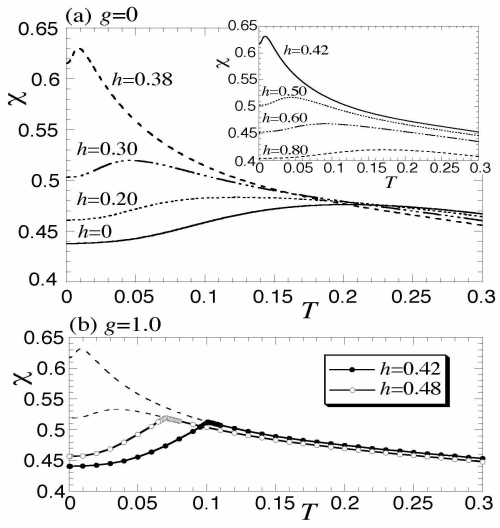

FIG. 3: T dependence of χ for several choices of h for $g = 0$ (a) and $g = 1.0$ (b); the dashed lines in (b) are data for $g = 0$; $h = 0.4$ corresponds to the van Hove energy of the up-spin band.

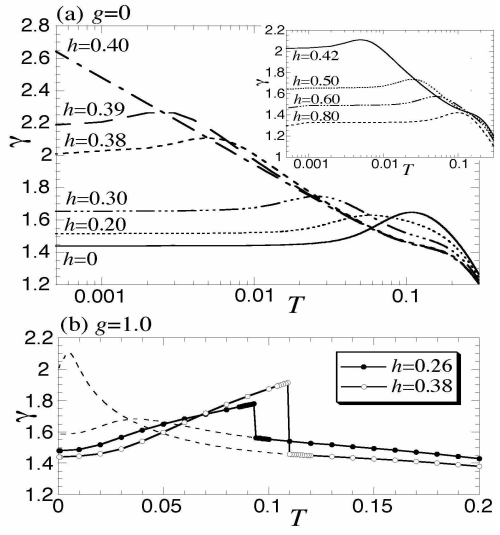

FIG. 4: T dependence of γ for several choices of h for $g = 0$ (a) and $g = 1.0$ (b); a logarithmic T scale is used in (a); the dashed lines in (b) are data for $g = 0$.